



Development of an Advanced Urban Dispersion Modeling Capability



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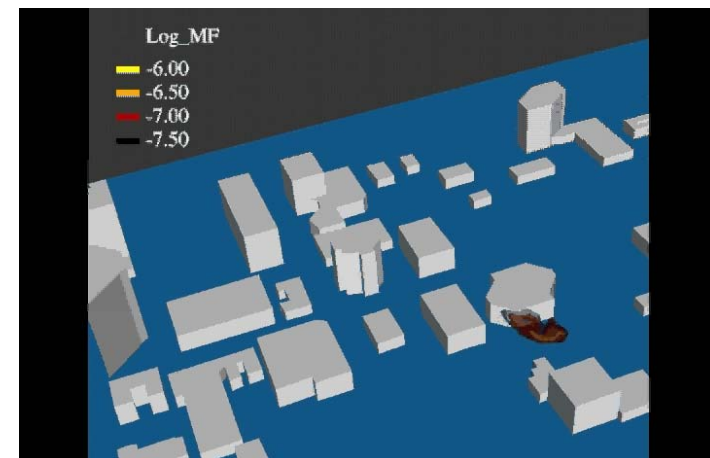
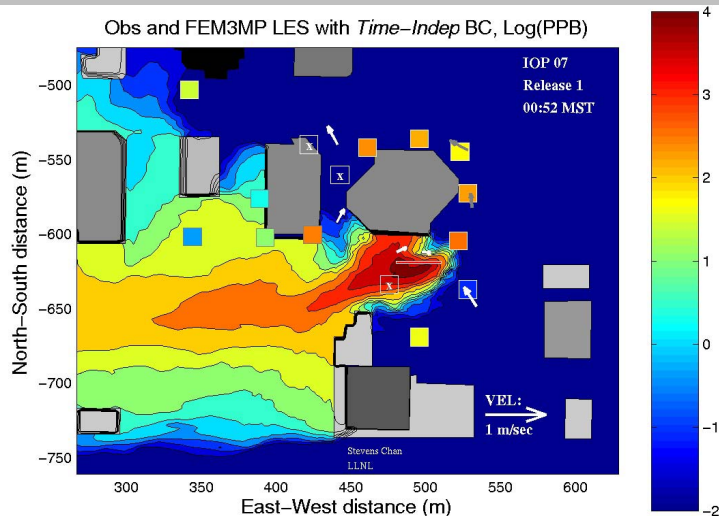


DHS PI Meeting
Lawrence Livermore National Lab
March 16-17, 2004

Accurate and timely prediction of atmospheric dispersion of hazardous materials is a critical national security need.



- **High-fidelity urban dispersion simulations are important:**
 - Experimental measurements alone are insufficient for emergency response and planning
 - Field experiments are expensive
 - Simulations are used to guide more effective sensor deployments
 - Together with measurements, simulations are an essential tool for event reconstruction

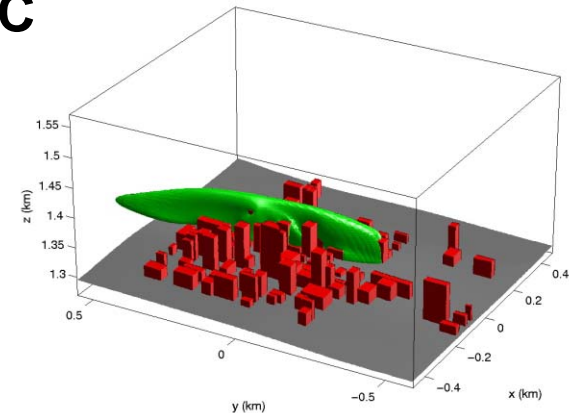


Urban dispersion modeling capabilities have been developed by researchers in NARAC



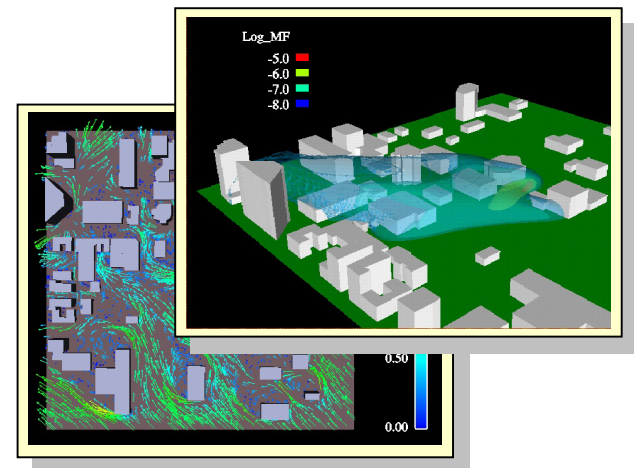
- The standalone **FEM3MP** code is the primary urban dispersion modeling code used in the atmospheric sciences division in NARAC

- Finite element incompressible CFD
- Structured mesh
- LES & RANS turbulence models
- Atmospheric chemistry



- Operational use limited due to

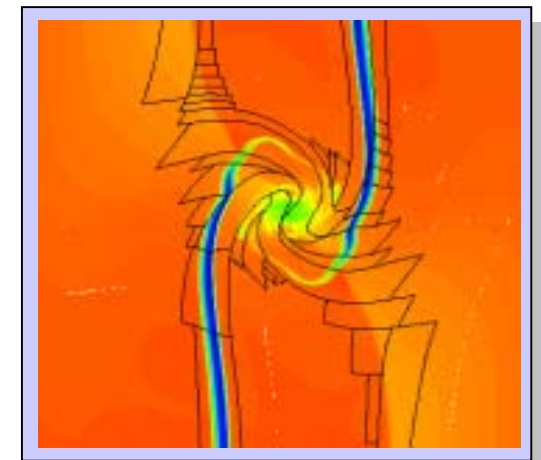
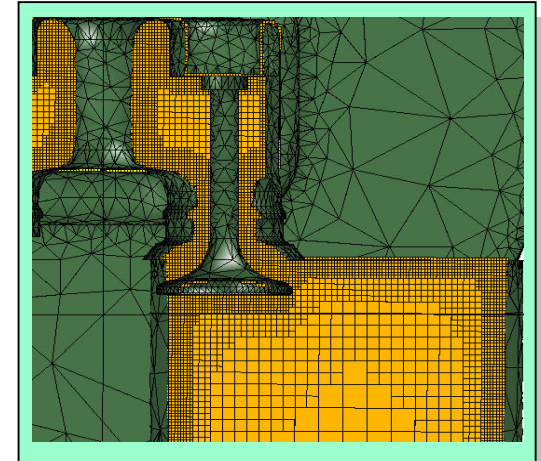
- Simple geometry representation
- Laborious grid generation
- Range of release scenarios (e.g. unable to simulate moving sources)



We propose to apply advanced meshing tools to the numerical models developed in NARAC



- The **Overture** project has tools for rapid geometry-to-mesh (Rapsodi) capability
 - Rapid construction of surface grids from CAD data
 - Interfaces to fast volume grid generator from NASA (CUBES)
- The **SAMRAI** infrastructure supports a variety of parallel AMR applications
 - Data structures for flexible mesh geometry
 - Adaptive mesh refinement
 - Scalability verified on > 1K processors



The coupled technologies will lead to an advanced operational capability



FEM3MP

Incompressible flow solver for urban dispersion applications

SAMRAI

Support for flexible mesh geometry:
Adaptive mesh refinement

Overture

Rapid geometry-to-mesh capability using building datasets

Next-generation State-of-the-art
Integrated Urban Dispersion Capability

- Automatic mesh construction from building datasets.
- Geometrically complex buildings and cityscapes
- Applicable to diverse urban environments: stadiums, arenas, subways, etc.

- Adaptive mesh refinement capability
- Enhanced fidelity around important flow regions: release source, building entrance, etc.
- Complex release scenarios: moving sources, etc.

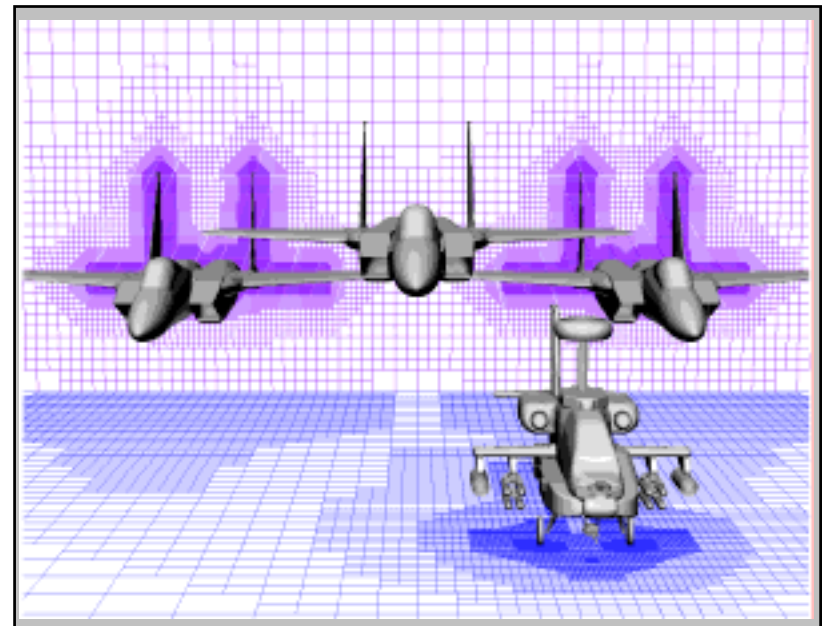
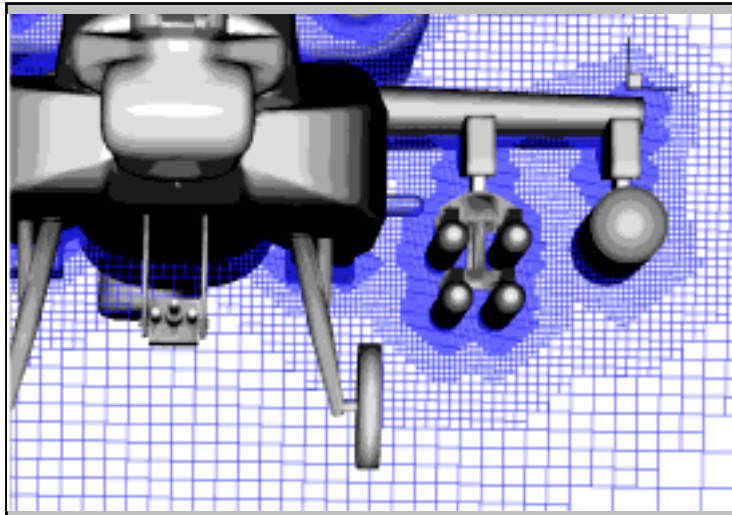
The CUBES software is used to build adaptive cut-cell volume grids



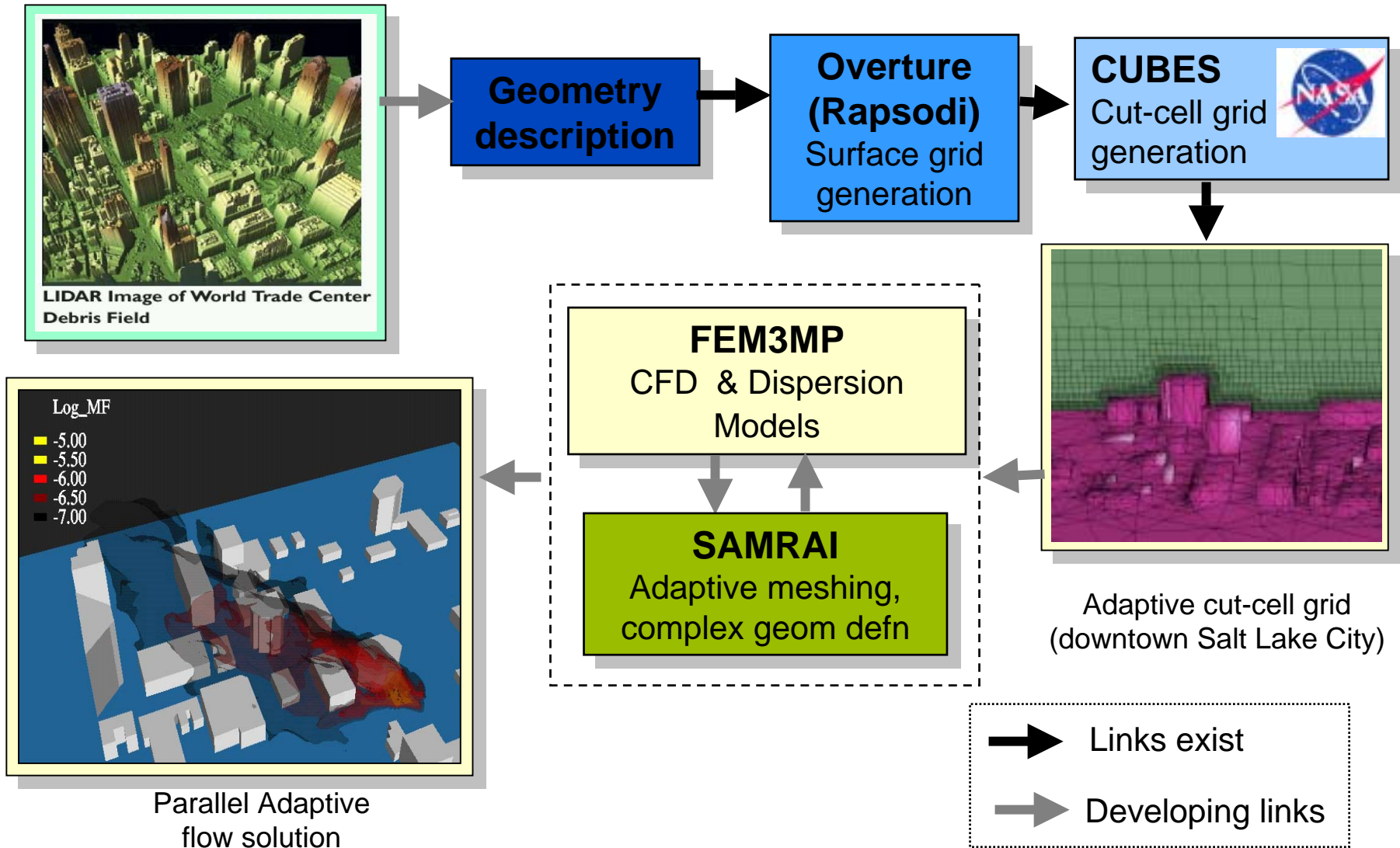
- **CUBES is a grid generator developed at NASA Ames for automated CFD analysis.**
 - Developed by Marsha Berger (NYU, Courant) and Mike Aftosmis (NASA Ames)
 - Readily handles complex geometries
 - Very fast



Example applications of CUBES –
courtesy Berger, Aftosmis NASA Ames



An integrated set of tools will provide rapid geometry to solution capability





Multidisciplinary Project Team

Technical team:

▪ Kyle Chand (Overture, CASC)	grid generation	25%
▪ Brian Gunney (SAMRAI, CASC)	AMR, numerical alg.	25%
▪ Craig Kapfer (SAMRAI, CASC)	AMR, software integ.	50%
▪ Branko Kosovic (FEM3MP, ASD)	atmospheric applic.	50%
▪ Anders Petersson (Overture, CASC)	grid generation	25%
▪ Andy Wissink (SAMRAI, CASC)	AMR, cut-cell grids	50%

Collaborator:

▪ Marsha Berger (NYU, Courant)	grid generation	(unfunded)
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Customers and Funding

We are funded by the Threat Vulnerability Test and Assessment (TVTA) portfolio in the DHS S&T program.

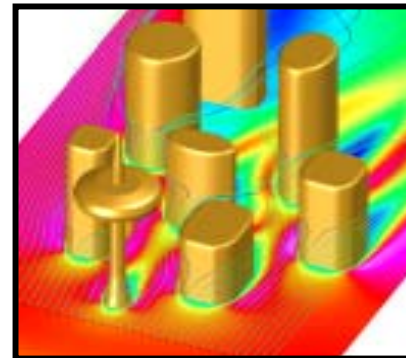
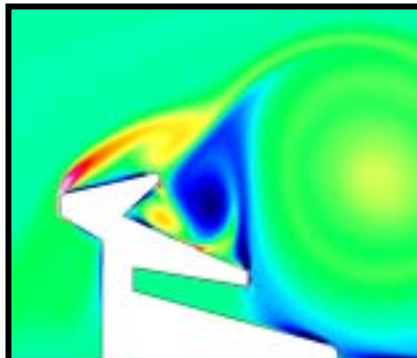
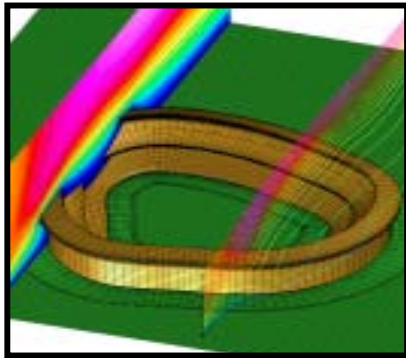
National Release Advisory Center (NARAC) will be the primary customer

- NARAC is a part of the Emergency Preparedness and Response program in the DHS
- Infrastructure and critical facility protection, vulnerability studies

Demonstration calculations with prototype problems – 9/03

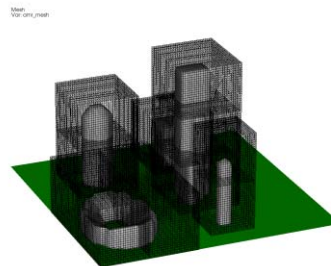
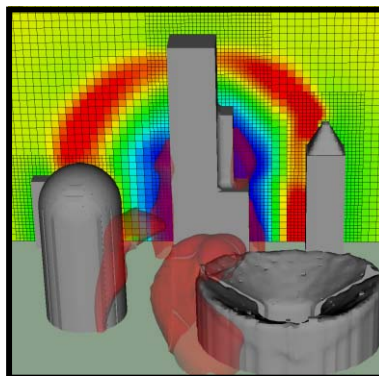


- Flow around stadium and sample cityscape with overset grids

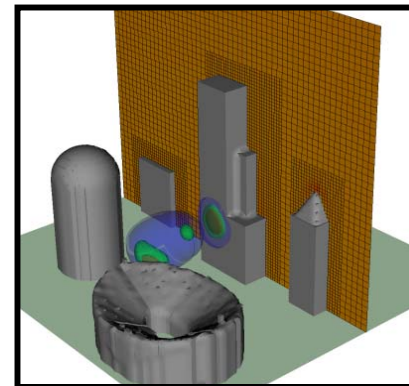


Henshaw 9/03

- Adaptive flow simulation over prototype cityscape with cut-cell grids



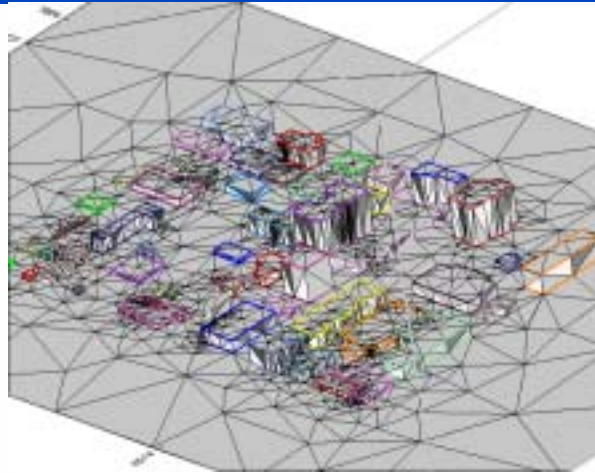
Refined region
around buildings



Automated cut-cell grid generation from building datasets – 1/04

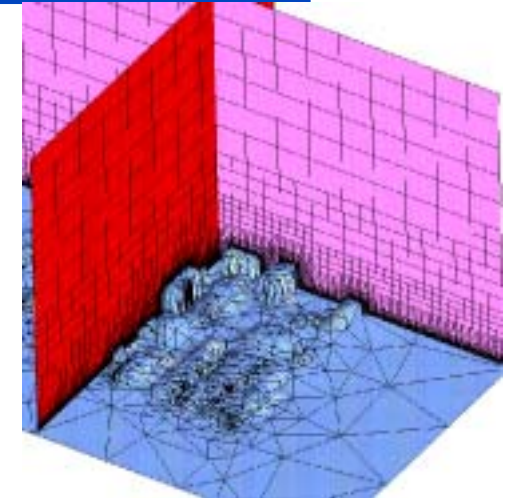


Polygonal geometry data (Salt Lake City)



Surface triangulation by
metro

Chand 1/04



AMR volume mesh
by **CUBES**

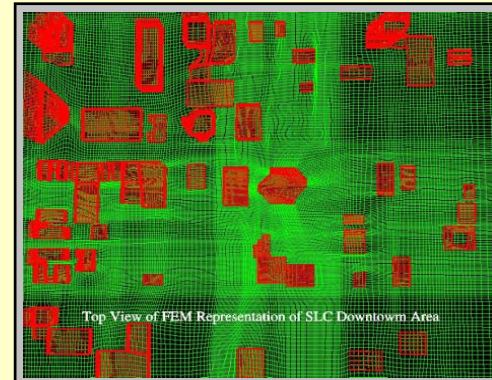
- “metro” reads building geometry data and generates surface triangulation and CUBES input
- GUI interface that allows user to interactively add/modify/delete buildings

Mesh generation with new tools is considerably faster than current tools



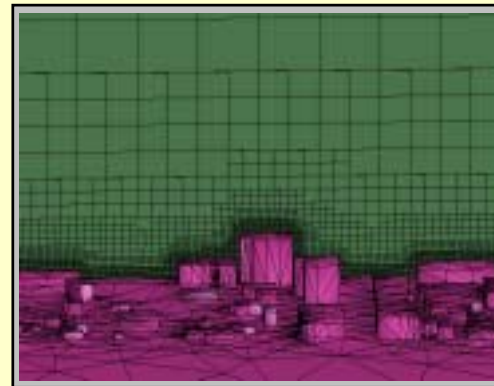
Downtown Salt Lake City

- Structured conforming grid constructed with existing tools required about a week



- Adaptive cut-cell Cartesian grid generated with metro & CUBES required about 2 minutes

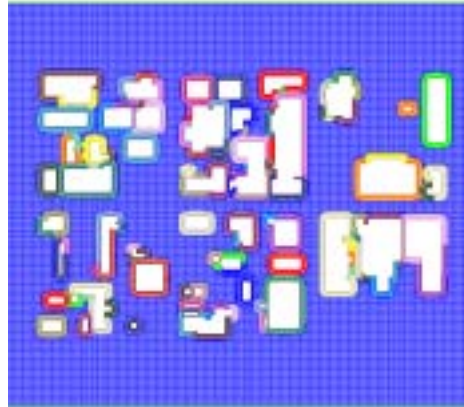
1.7M gridpoints, 6 levels refinement
Surface grid – 30 sec with “metro”
Volume grid – 45 sec with “CUBES”



Automated overlapping grid construction from building geometry information



Polygonal geometry
data (Salt Lake City)



2D overlapping grid
(ogen)



Henshaw 1/04

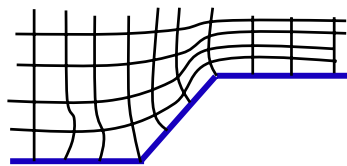
INS Solution
(Overblown)

- **Body-fitted grids are automatically generated for each building**
- **Cartesian grid fills background and far-field**
- **Overlapping grid is automatically assembled**

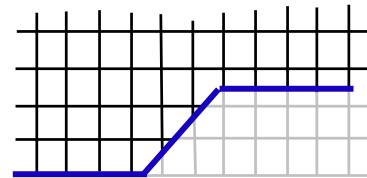


Research issues still to be addressed in FY04

- **Finite element boundary representation on cut-cell grids – fictitious domain**



“conforming” mesh
(current)



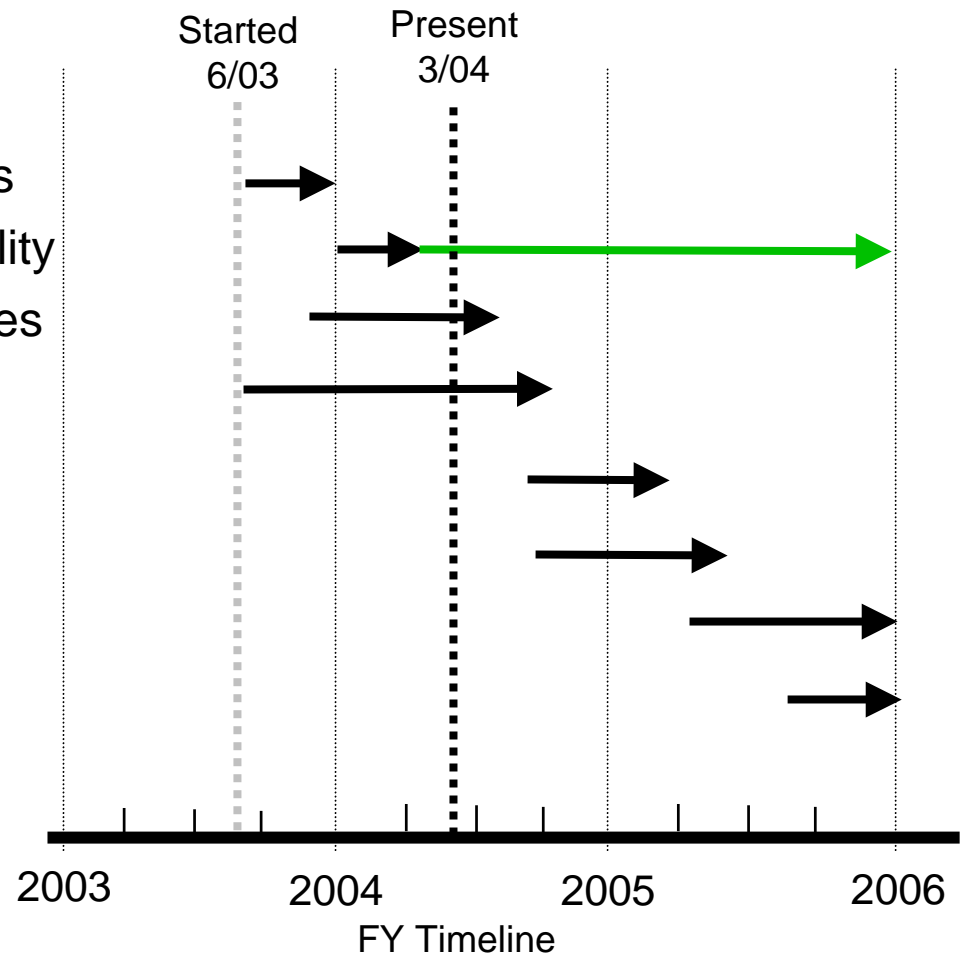
“cut-cell” mesh
(new)

- **Adaptive algorithms for Q1Q0 and Q1Q1 element incompressible CFD solver**
- **Building geometry information that incorporates new features**
 - Standard formats adopted by DHS?
 - Incorporating terrain



Project Tasks and Timeline

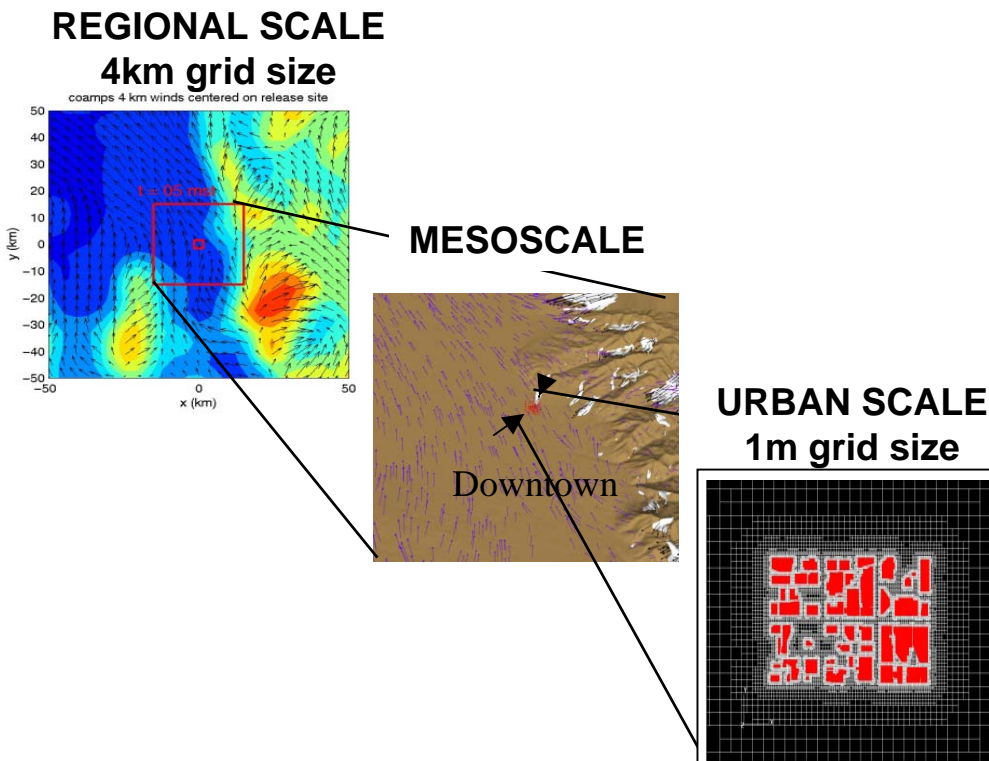
- Demonstration calc with prototypes
- Develop geometry to mesh capability
- Develop CUBES/SAMRAI interfaces
- SAMRAI-FEM3MP integration
- Develop cut-cell FE algs
- Develop AMR capability
- Validation, refinement studies
- Fine-tune the performance for operational use





Potential Longer-term Research Challenges

- Coupling models with different scales
- Diverse urban environments – subways, arenas, etc.



- Large-scale cityscapes (e.g. Manhattan)
- Performance on diverse parallel architectures



Conclusions

- **We are pursuing an advanced urban dispersion modeling tool by combining expertise in meshing technologies from CASC and NASA with atmospheric model expertise in NARAC.**
- **The tool will be used for emergency response, scenerio planning, and event reconstruction capability**
- **Our grid generation approach demonstrates it is possible to reduce meshing times from weeks to minutes.**
- **Anticipate fully adaptive tool to be available for operational use in NARAC by late 2005.**



Acknowledgments

- This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.
- Document UCRL-PRES-202875